

1-Methylpyrene
2381-21-7 | DTXSID0025654

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1360

Global applicability domain: Inside

Local applicability domain index: 4.39e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,5,9-Cyclododecatiene

Measured: 8320

Predicted: 4560

[Image not found](#)

2,2,4,6,6-Pentamethylheptane

Measured: 871

Predicted: 963

[Image not found](#)

4-(1,1,3,3-Tetramethylbutyl)phenol

Measured: 288

Predicted: 134

[Image not found](#)

Isobutyl 2-naphthyl ether

Measured: 631

Predicted: 136